

Message

From: Evich, Marina [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=7076C6258190415D9B36A76D03FE3313-EVICH, MARI]
Sent: 5/18/2020 6:59:11 PM
To: Washington, John [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=fdc3e8ce9f1d45c4894881ff420ca104-Washington, John]
Subject: RE: CIPFPECA degradation search on GC/MS
Attachments: NJ_degradation-QTOF peak areas2.xlsx

Sure, sorry I wasn't being clear. 3:30-3:45 sounds ok. I've attached a spreadsheet as well.

From: Washington, John <Washington.John@epa.gov>
Sent: Monday, May 18, 2020 2:53 PM
To: Evich, Marina <evich.marina@epa.gov>
Subject: RE: CIPFPECA degradation search on GC/MS

Hi Marina,

This sounds great. I am not sure I understand a few parts. Mind if I call you at about 3:30 to 3:45? Should I have your Powerpoint open, or Eric's from today?

Thanks,
John

From: Evich, Marina <evich.marina@epa.gov>
Sent: Monday, May 18, 2020 2:00 PM
To: Washington, John <Washington.John@epa.gov>; Henderson, Matt <Henderson.Matt@epa.gov>; Acrey, Brad <Acrey.Brad@epa.gov>
Cc: Weber, Eric <Weber.Eric@epa.gov>; Davis, Mary J. <davis.maryj@epa.gov>; Stevens, Caroline <Stevens.Caroline@epa.gov>
Subject: RE: CIPFPECA degradation search on GC/MS

Hi John,

I don't have much experience with GC/MS, but I think that looking for the suspected new products by GC/MS could be interesting. Just looking at MSe data by LC-MS, I'm seeing masses that correspond to the Cl-PFPECA (-COOH) for (0,1), aka, the decarboxylated chlorinated precursor in some of the samples including veg8, veg1, and SC1 – but these have not been confirmed with MSMS. The only possibly decarboxylated degradation product I am seeing in MSe data is the decarboxylated u-product (that first unsaturated decarboxylated product $C_7F_{13}O_2^-$) and the 3rd degradation product, the decarboxylated diOH-product ($C_7F_{13}O_4H_2^-$) in SS4. Eric, do you also suspect a Cl loss (Cl->H) decarboxylated product?

I don't know where the soil samples are kept, but I think that SS8, SS4 and SC1 would be good samples to start with if Matt thinks these would be good GC/MS candidates. I also think it's a good idea to do the extractions in replicates. Brad, would you be ok with doing the MTBE/water extraction? We can work on the extraction together.

Marina

From: Washington, John <Washington.John@epa.gov>
Sent: Monday, May 18, 2020 11:24 AM
To: Evich, Marina <evich.marina@epa.gov>; Henderson, Matt <Henderson.Matt@epa.gov>; Acrey, Brad <Acrey.Brad@epa.gov>

Cc: Weber, Eric <Weber.Eric@epa.gov>; Davis, Mary J. <davis.maryj@epa.gov>; Stevens, Caroline <Stevens.Caroline@epa.gov>

Subject: CIPFPECA degradation search on GC/MS

Hello everyone,

Marina is leading our effort to find degradation products of the chloro perfluoro polyether carboxylates (CIPFPECAs) that we have found in New Jersey soils. So far Marina has tentatively identified several generations of degradants initiated at reductive loss of Cl.

Our esteemed colleague and renowned polymath, Eric suspects that these CIPFPECAs also might degrade by loss of the carboxylate. Unfortunately, ESI ionization on LC causes in-source loss of the carboxylate, so LC is not a good analytical tool for detecting this hypothetical carboxylate loss.

If you look at Eric's proposed scheme (attached), I suspect the first four generations of carboxylate-loss products might be detected on GC/MS in PCI with the M+1 mass – Matt, what do you think? Is it worth extracting a NJ soil for GC/MS and running PCI on GC/MS plus a nontargeted scan on GC/QToF in whatever mode you say? Then extracting exact masses because they likely will be minor signals if present at all?

Marina should continue being lead on this, so Marina:

1. Do you want me to find the soils to extract – if so, are SS8 and SS4 the ones you like? Or do you know where they are???
2. Do you want Brad to run the MTBE/water extractions that we have had success with in the past for GC/MS analytes? OK Brad?
3. If so, do you want triplicate extraction of each soil sample? (Don't you have variability among reps in the clarity of your detections???)
4. Then you coordinate with Matt on the analyses, e.g., GC-PCI/MS and GC-QToF? OK Matt?

Also Marina, I notice the last two generations of carboxylate degradants that Eric proposes look as though they might be detectable on LC-ToF (acids). Might be worth a look at your MSe data.

Just thoughts to start the conversation,
John

From: Weber, Eric <Weber.Eric@epa.gov>

Sent: Monday, May 18, 2020 9:31 AM

To: Washington, John <Washington.John@epa.gov>

Subject: RE: 5/26 CSS Science Webinar

Currently working on the degradation pathways of the chlorinated carboxy ethers. The first one is attached. More explanation of the pathways to follow.

Eric